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data_lach13

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 'C59 H127 N4 Na O37.50 P3 Si W9'
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 'Si'  'Si'   0.0817   0.0704
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 'x, x-y, z+1/2'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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^)/3'
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H1A H -0.1593 0.7280 0.8617 0.074 Uiso 1 1 calc R . .
H1B H -0.1306 0.7034 0.8264 0.074 Uiso 1 1 calc R . .
C2 C -0.0658(8) 0.7324(10) 0.8738(5) 0.071(5) Uani 1 1 d D . .
H2A H -0.0564 0.7545 0.8981 0.085 Uiso 1 1 calc R . .
C3 C -0.0338(10) 0.6971(10) 0.8642(7) 0.091(8) Uani 1 1 d . . .
H3A H -0.0426 0.6747 0.8400 0.109 Uiso 1 1 calc R . .
H3B H -0.0022 0.6945 0.8816 0.109 Uiso 1 1 calc R . .
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C4 C 0.1654(8) 0.8718(7) 0.8199(4) 0.048(3) Uani 1 1 d D . .
H4A H 0.1172 0.8422 0.8107 0.058 Uiso 1 1 calc R . .
H4B H 0.1810 0.9200 0.8116 0.058 Uiso 1 1 calc R . .
C5 C 0.1645(8) 0.8701(8) 0.8637(4) 0.052(3) Uani 1 1 d D . .
H5A H 0.2127 0.8961 0.8736 0.062 Uiso 1 1 calc R . .
H5B H 0.1431 0.8214 0.8727 0.062 Uiso 1 1 calc R . .
C6 C 0.1227(9) 0.9031(9) 0.8782(5) 0.061(4) Uani 1 1 d D . .
H6A H 0.1426 0.9507 0.8678 0.074 Uiso 1 1 calc R . .
H6B H 0.0740 0.8754 0.8693 0.074 Uiso 1 1 calc R . .
C7 C 0.1243(12) 0.9058(12) 0.9217(5) 0.088(7) Uani 1 1 d D . .
H7A H 0.0972 0.9268 0.9308 0.132 Uiso 1 1 calc R . .
H7B H 0.1725 0.9339 0.9305 0.132 Uiso 1 1 calc R . .
H7C H 0.1043 0.8586 0.9320 0.132 Uiso 1 1 calc R . .
C8 C 0.2864(7) 0.8915(7) 0.8146(5) 0.058(4) Uani 1 1 d D . .
H8A H 0.2878 0.8822 0.8423 0.069 Uiso 1 1 calc R . .
H8B H 0.3149 0.8755 0.8010 0.069 Uiso 1 1 calc R . .
C9 C 0.3193(7) 0.9699(7) 0.8089(5) 0.060(4) Uani 1 1 d D . .
H9A H 0.3138 0.9799 0.7819 0.072 Uiso 1 1 calc R . .
H9B H 0.2955 0.9879 0.8254 0.072 Uiso 1 1 calc R . .
C10 C 0.3959(7) 1.0058(8) 0.8191(6) 0.072(5) Uani 1 1 d D . .
H10A H 0.4197 0.9883 0.8022 0.087 Uiso 1 1 calc R . .
H10B H 0.4013 0.9946 0.8459 0.087 Uiso 1 1 calc R . .
C11 C 0.4301(11) 1.0849(8) 0.8146(7) 0.092(7) Uani 1 1 d D . .
H11A H 0.4175 1.0957 0.7897 0.138 Uiso 1 1 calc R . .
H11B H 0.4807 1.1060 0.8162 0.138 Uiso 1 1 calc R . .
H11C H 0.4138 1.1036 0.8350 0.138 Uiso 1 1 calc R . .
C12 C 0.2049(7) 0.8562(7) 0.7579(4) 0.044(3) Uani 1 1 d D . .
H12A H 0.2151 0.9043 0.7528 0.053 Uiso 1 1 calc R . .
H12B H 0.1563 0.8243 0.7500 0.053 Uiso 1 1 calc R . .
C13 C 0.2525(7) 0.8419(8) 0.7331(4) 0.053(4) Uani 1 1 d D . .
H13A H 0.2430 0.7939 0.7377 0.064 Uiso 1 1 calc R . .
H13B H 0.3016 0.8744 0.7400 0.064 Uiso 1 1 calc R . .
C14 C 0.2411(8) 0.8508(8) 0.6904(4) 0.063(4) Uani 1 1 d D . .
H14A H 0.1916 0.8190 0.6839 0.076 Uiso 1 1 calc R . .
H14B H 0.2510 0.8990 0.6861 0.076 Uiso 1 1 calc R . .
C15 C 0.2865(9) 0.8361(11) 0.6637(6) 0.094(7) Uani 1 1 d D . .
H15A H 0.2773 0.8429 0.6371 0.141 Uiso 1 1 calc R . .
H15B H 0.2759 0.7879 0.6673 0.141 Uiso 1 1 calc R . .
H15C H 0.3356 0.8678 0.6697 0.141 Uiso 1 1 calc R . .
C16 C 0.1866(6) 0.7717(6) 0.8101(4) 0.049(3) Uani 1 1 d D . .
H16A H 0.2175 0.7587 0.7966 0.059 Uiso 1 1 calc R . .
H16B H 0.1931 0.7684 0.8379 0.059 Uiso 1 1 calc R . .
C17 C 0.1119(6) 0.7186(6) 0.8002(4) 0.053(4) Uani 1 1 d D . .
H17A H 0.0833 0.7413 0.8011 0.063 Uiso 1 1 calc R . .
H17B H 0.0936 0.6812 0.8197 0.063 Uiso 1 1 calc R . .
C18 C 0.1045(7) 0.6862(6) 0.7605(4) 0.056(4) Uani 1 1 d DU . .
H18A H 0.1391 0.6709 0.7574 0.067 Uiso 1 1 calc R . .
H18B H 0.1128 0.7209 0.7403 0.067 Uiso 1 1 calc R . .
C19 C 0.0300(9) 0.6232(8) 0.7566(7) 0.086(6) Uani 1 1 d DU . .
H19A H 0.0245 0.6019 0.7313 0.130 Uiso 1 1 calc R . .
H19B H -0.0039 0.6388 0.7596 0.130 Uiso 1 1 calc R . .
H19C H 0.0223 0.5889 0.7765 0.130 Uiso 1 1 calc R . .
C20 C 0.0154(17) 0.9577(12) 1.025(3) 0.33(5) Uani 0.33 1 d PDU . .
C21 C 0.037(2) 0.9021(18) 1.021(5) 0.32(5) Uani 0.33 1 d PDU . .
H21A H 0.0880 0.9248 1.0196 0.481 Uiso 0.33 1 calc PR . .
H21B H 0.0166 0.8742 0.9980 0.481 Uiso 0.33 1 calc PR . .
H21C H 0.0210 0.8718 1.0437 0.481 Uiso 0.33 1 calc PR . .
N1 N 0.2106(6) 0.8482(6) 0.8007(4) 0.049(3) Uani 1 1 d D . .
N2 N 0.0000 1.0000 1.026(3) 0.33(4) Uani 1 3 d SDU . .
O1 O 0.0959(4) 0.9279(4) 0.7574(2) 0.0301(16) Uani 1 1 d . . .
O2 O -0.0182(4) 0.8313(4) 0.8010(3) 0.0364(18) Uani 1 1 d . . .
O3 O 0.0315(4) 0.7866(4) 0.7418(3) 0.0379(19) Uani 1 1 d . . .
O4 O -0.0890(4) 0.7926(4) 0.7356(2) 0.0301(16) Uani 1 1 d . . .
O5 O -0.1377(4) 0.8198(4) 0.7993(3) 0.0366(18) Uani 1 1 d . . .
O6 O -0.2256(4) 0.7633(4) 0.7372(3) 0.0368(19) Uani 1 1 d . . .
O7 O -0.0355(3) 0.9197(4) 0.7545(3) 0.0289(16) Uani 1 1 d . . .

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O8 O 0.0000 1.0000 0.6946(4) 0.028(3) Uani 1 3 d SU . .
O9 O 0.0192(4) 0.8798(4) 0.6944(2) 0.0310(17) Uani 1 1 d . . .
O10 O 0.1287(4) 0.9988(4) 0.6939(2) 0.0305(16) Uani 1 1 d . . .
O11 O 0.0864(4) 0.9218(4) 0.6247(3) 0.0386(19) Uani 1 1 d . . .
O12 O -0.0378(4) 0.9188(4) 0.6367(2) 0.0308(16) Uani 1 1 d . . .
O13 O -0.0569(6) 0.8772(7) 0.8565(3) 0.058(3) Uani 1 1 d . . .
O14 O 0.0000 1.0000 0.931(4) 0.24(7) Uani 0.47(14) 3 d SPU . .
Na1 Na 0.0000 1.0000 0.8698(5) 0.087(4) Uani 1 3 d S . .
Si1 Si 0.0000 1.0000 0.74231(14) 0.0196(8) Uani 1 3 d S . .
P1 P -0.07945(17) 0.82450(18) 0.82629(11) 0.0390(7) Uani 1 1 d . . .
W1 W 0.00890(2) 0.84926(2) 0.746752(13) 0.02949(11) Uani 1 1 d . . .
W2 W -0.14413(2) 0.83497(2) 0.743403(13) 0.02923(10) Uani 1 1 d . . .
W3 W 0.05192(2) 0.95164(2) 0.657757(17) 0.02797(9) Uani 1 1 d . . .

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C2 0.062(10) 0.077(12) 0.070(12) 0.031(10) 0.011(9) 0.032(9)
C3 0.059(10) 0.086(13) 0.14(2) 0.057(14) 0.028(11) 0.048(10)
C4 0.059(8) 0.045(7) 0.053(9) 0.007(6) -0.002(7) 0.035(6)
C5 0.053(8) 0.050(8) 0.055(10) 0.002(7) -0.006(7) 0.028(6)
C6 0.062(9) 0.068(10) 0.062(11) -0.001(8) -0.001(8) 0.039(8)
C7 0.090(15) 0.098(15) 0.058(13) -0.016(11) -0.008(11) 0.033(12)
C8 0.049(8) 0.067(9) 0.069(11) 0.013(8) -0.015(7) 0.037(7)
C9 0.055(8) 0.050(8) 0.075(11) 0.008(7) -0.019(8) 0.026(7)
C10 0.043(8) 0.066(10) 0.096(15) 0.026(10) -0.009(8) 0.017(7)
C11 0.082(14) 0.068(12) 0.12(2) -0.010(12) -0.006(13) 0.033(11)
C12 0.046(7) 0.046(7) 0.047(8) 0.005(6) -0.005(6) 0.028(6)
C13 0.035(6) 0.056(8) 0.079(11) 0.024(8) 0.011(6) 0.030(6)
C14 0.049(8) 0.049(8) 0.094(14) 0.011(8) 0.010(8) 0.026(7)
C15 0.055(11) 0.086(15) 0.14(2) 0.020(14) 0.030(12) 0.033(11)
C16 0.051(7) 0.029(5) 0.073(11) 0.006(6) -0.006(7) 0.024(5)
C17 0.053(8) 0.035(6) 0.072(11) 0.007(6) -0.008(7) 0.024(6)
C18 0.053(8) 0.034(6) 0.078(11) 0.003(6) -0.016(7) 0.019(6)
C19 0.083(13) 0.041(8) 0.112(17) -0.002(9) -0.028(12) 0.014(8)
C20 0.34(5) 0.34(5) 0.32(6) 0.00(2) 0.000(19) 0.17(3)
C21 0.33(6) 0.32(6) 0.31(7) 0.03(4) -0.01(4) 0.16(4)
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N2 0.34(5) 0.34(5) 0.32(6) 0.000 0.000 0.17(3)
O1 0.030(3) 0.029(3) 0.039(5) -0.003(3) -0.004(3) 0.020(3)
O2 0.037(4) 0.033(4) 0.042(5) 0.005(3) -0.003(4) 0.019(3)
O3 0.033(4) 0.031(4) 0.055(6) 0.002(4) 0.000(4) 0.019(3)
O4 0.038(4) 0.019(3) 0.036(4) 0.004(3) 0.008(3) 0.016(3)
O5 0.026(3) 0.029(4) 0.050(5) 0.002(3) 0.010(3) 0.011(3)
O6 0.021(3) 0.031(4) 0.054(6) -0.007(4) 0.004(3) 0.009(3)
O7 0.020(3) 0.028(3) 0.036(4) -0.005(3) -0.002(3) 0.010(3)
O8 0.024(3) 0.024(3) 0.036(8) 0.000 0.000 0.0119(17)
O9 0.026(3) 0.023(3) 0.044(5) 0.000(3) 0.003(3) 0.013(3)
O10 0.023(3) 0.028(3) 0.041(5) 0.001(3) 0.005(3) 0.014(3)
O11 0.038(4) 0.039(4) 0.044(5) -0.002(4) 0.003(4) 0.024(4)
O12 0.032(4) 0.025(3) 0.033(4) -0.002(3) -0.001(3) 0.012(3)
O13 0.065(7) 0.074(7) 0.052(7) -0.005(6) 0.002(5) 0.048(6)
O14 0.29(8) 0.29(8) 0.13(9) 0.000 0.000 0.15(4)
Na1 0.075(6) 0.075(6) 0.112(13) 0.000 0.000 0.038(3)
Si1 0.0241(12) 0.0241(12) 0.0106(19) 0.000 0.000 0.0121(6)
P1 0.0342(14) 0.0426(16) 0.0439(19) 0.0107(14) 0.0067(13) 0.0221(13)
W1 0.02638(18) 0.02197(17) 0.0416(3) 0.00213(16) 0.00136(18) 0.01320
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W2 0.02255(17) 0.02151(17) 0.0402(3) 0.00133(17) 0.00104(17) 0.00844
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C1 P1 1.816(15) . ?
C2 C3 1.34(2) . ?
C4 N1 1.503(14) . ?
C4 C5 1.527(15) . ?
C5 C6 1.530(15) . ?
C6 C7 1.519(16) . ?
C8 C9 1.528(15) . ?
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C17 C18 1.532(15) . ?
C18 C19 1.548(15) . ?
C20 N2 1.1502(10) . ?
C20 C21 1.5402(11) . ?
N2 C20 1.1502(11) 3_465 ?
N2 C20 1.1502(13) 2_675 ?
O1 W1 1.883(7) . ?
O1 W2 1.922(7) 2_675 ?
O2 P1 1.565(9) . ?
O2 W1 1.967(9) . ?
O3 W1 1.707(8) . ?
O4 W2 1.899(7) . ?
O4 W1 1.930(8) . ?
O5 P1 1.561(10) . ?
O5 W2 1.998(10) . ?
O6 W2 1.725(7) . ?
O7 Si1 1.605(8) . ?
O7 W2 2.230(7) . ?
O7 W1 2.244(7) . ?
O8 Si1 1.666(16) . ?
O8 W3 2.319(8) 3_465 ?
O8 W3 2.319(8) . ?
O8 W3 2.319(8) 2_675 ?
O9 W3 1.884(8) . ?
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O9 W1 1.924(9) . ?
O10 W2 1.864(8) 2_675 ?
O10 W3 1.954(8) . ?
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O13 P1 1.465(12) . ?
O13 Na1 2.409(13) . ?
Na1 O13 2.409(13) 2_675 ?
Na1 O13 2.409(13) 3_465 ?
Si1 O7 1.605(8) 2_675 ?
Si1 O7 1.605(8) 3_465 ?
W2 O10 1.864(8) 3_465 ?
W2 O1 1.922(7) 3_465 ?
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C7 C6 C5 110.2(15) . . ?
C9 C8 N1 114.9(10) . . ?
C10 C9 C8 109.9(11) . . ?
C9 C10 C11 111.1(14) . . ?
N1 C12 C13 115.4(10) . . ?
C12 C13 C14 110.4(10) . . ?
C15 C14 C13 113.1(14) . . ?
C17 C16 N1 116.7(10) . . ?
C16 C17 C18 113.0(11) . . ?
C17 C18 C19 108.5(13) . . ?
N2 C20 C21 177(3) . . ?
C4 N1 C12 106.9(9) . . ?
C4 N1 C8 110.6(12) . . ?
C12 N1 C8 111.6(12) . . ?
C4 N1 C16 111.3(11) . . ?
C12 N1 C16 109.8(10) . . ?
C8 N1 C16 106.8(9) . . ?
C20 N2 C20 119.9(7) 3_465 2_675 ?
C20 N2 C20 119.9(8) 3_465 . ?
C20 N2 C20 119.9(8) 2_675 . ?
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P1 O2 W1 136.5(5) . . ?
W2 O4 W1 116.3(4) . . ?
P1 O5 W2 134.8(5) . . ?
Si1 O7 W2 127.9(4) . . ?
Si1 O7 W1 126.8(4) . . ?
W2 O7 W1 93.3(3) . . ?
Si1 O8 W3 123.7(3) . 3_465 ?
Si1 O8 W3 123.7(3) . . ?
W3 O8 W3 92.2(4) 3_465 . ?
Si1 O8 W3 123.7(3) . 2_675 ?
W3 O8 W3 92.2(4) 3_465 2_675 ?
W3 O8 W3 92.2(4) . 2_675 ?
W3 O9 W1 150.6(4) . . ?
W2 O10 W3 152.5(4) 2_675 . ?
W3 O12 W3 120.8(4) . 3_465 ?
P1 O13 Na1 145.1(9) . . ?
O13 Na1 O13 116.4(3) 2_675 . ?
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O7 Si1 O7 113.2(3) 2_675 3_465 ?
O7 Si1 O7 113.2(3) . 3_465 ?
O7 Si1 O8 105.4(4) 2_675 . ?
O7 Si1 O8 105.4(4) . . ?
O7 Si1 O8 105.4(4) 3_465 . ?
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O13 P1 O2 113.3(6) . . ?
O5 P1 O2 108.5(5) . . ?
O13 P1 C1 110.3(9) . . ?
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O2 P1 C1 104.2(6) . . ?
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O3 W1 O2 96.8(4) . . ?
O1 W1 O2 93.8(4) . . ?
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O4 W1 O2 86.1(3) . . ?
O3 W1 O7 172.3(3) . . ?
O1 W1 O7 86.2(3) . . ?
O9 W1 O7 83.4(3) . . ?
O4 W1 O7 74.6(3) . . ?
O2 W1 O7 80.1(3) . . ?
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O6 W2 O4 99.4(3) . . ?
O10 W2 O4 94.0(3) 3_465 . ?
O6 W2 O1 100.8(3) . 3_465 ?
O10 W2 O1 86.8(3) 3_465 3_465 ?
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O6 W2 O5 95.6(4) . . ?
O10 W2 O5 165.2(3) 3_465 . ?
O4 W2 O5 86.5(3) . . ?
O1 W2 O5 87.6(3) 3_465 . ?
O6 W2 O7 173.7(3) . . ?
O10 W2 O7 85.3(3) 3_465 . ?
O4 W2 O7 75.5(3) . . ?
O1 W2 O7 84.0(3) 3_465 . ?
O5 W2 O7 80.4(3) . . ?
O11 W3 O9 100.9(4) . . ?
O11 W3 O12 100.3(4) . . ?
O9 W3 O12 92.9(3) . . ?
O11 W3 O12 99.9(4) . 2_675 ?
O9 W3 O12 158.2(3) . 2_675 ?
O12 W3 O12 89.6(5) . 2_675 ?
O11 W3 O10 101.9(4) . . ?
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O12 W3 O10 157.8(3) . . ?
O12 W3 O10 86.4(3) 2_675 . ?
O11 W3 O8 170.6(4) . . ?
O9 W3 O8 86.9(3) . . ?
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